

WE CLAIM:

- 5 1. A computer-assisted method for determining a three-dimensional structure of a target amino acid sequence using a computer comprising a processor configured to receive and output data in accordance with executable code, the method comprising:
- (a) generating input data for the computer comprising:
 - (i) inputting into the computer an alignment of a target amino
 - 10 acid sequence with a template amino acid sequence; and
 - (ii) by way of executable code, directing the processor to produce from the alignment a three dimensional reduced protein model comprised of representations of side chains of amino acid residues comprising a target protein; and
 - 15 (b) outputting the three-dimensional reduced protein model to an output device or a storage device.
2. A method according to claim 1 wherein the executable code comprises instructions for:
- 20 (a) converting representations of the side chains of amino acid residues of the target protein to interaction centers connected by virtual covalent bonds, wherein each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds, and wherein each interaction center, except for the interaction centers
 - 25 representing the amino and carboxy terminal amino acid residues of the target protein, is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an interaction center chain; and
 - (b) projecting the interaction center chain onto an underlying cubic
 - 30 lattice to produce a projected chain of interaction centers;

- 5 (c) applying secondary constraints and/or tertiary constraints to a subset of interaction centers of the interaction center chain so as to produce a data set representing a three-dimensional model structure of the target protein.
- 10 3. A method according to claim 2 further comprising iterating steps (a)-(c), wherein in each iteration, a different set of secondary and tertiary constraints are applied to the interaction centers to produce a series of data sets representing three-dimensional model structures of the target protein, and wherein an energy computation is made for each member of the series of data sets representing the three-dimensional model structures of the target protein.
- 15 4. A method according to claim 3 further comprising selecting the member of the series of data sets representing the three-dimensional model structures of the target protein that has the lowest energy.
- 20 5. A method according to claim 4 wherein the data set representing the three-dimensional model structure of the target protein having the lowest energy is output to the data storage system to produce a stored data set.
- 25 6. A method according to claim 4 wherein the data set representing the three-dimensional model structure of the target protein having the lowest energy is output to an output device.
- 30 7. A method according to 5 wherein the stored data set is retrieved and displayed on an output device in a manner that allows the three-dimensional model structure of the target protein to be visualized.
8. A method according to claim 1 wherein the threading alignment input into the computer is retrieved from a data storage system.

- 5 9. A computer-assisted method for determining a three-dimensional structure of a target protein using a computer comprising a processor configured to receive and output data in accordance with executable code, the method comprising:
- (a) generating input data for the computer comprising:
 - (i) inputting as a string of an identity constraint and a secondary
10 structure constraint and/or tertiary constraints for some or all of the amino acid residues residue comprising the target protein; and
 - (ii) by way of executable code, directing the processor to produce
15 from the string a three dimensional reduced protein model comprised of representations of side chains of the amino acid residues comprising the target protein; and
 - (b) outputting the three dimensional reduced protein model to an output
20 device or a storage device.
10. A method according to claim 9 wherein the secondary structure constraint for each amino acid residue is selected from the group of "H" for helix, "E" for
25 extended, and "(-)" for other structural constraints.
11. A method according to claim 9 wherein the secondary structural constraint for a subset of amino acid residues comprising the target protein is generated by a
30 threading alignment of an amino acid sequence of the target protein.
12. A computer-assisted method for determining a three-dimensional structure of a target amino acid sequence, the method comprising inputting into the computer an alignment of a target amino acid sequence with a template amino acid sequence and
35 calculating with the said computer one or more three-dimensional reduced protein model comprising representations of side chains of amino acid residues comprising a target protein.